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Crystal structures of the potassium and rubidium salts of (3,5-dichlorophenoxy)acetic acid: two isotypic coordination polymers

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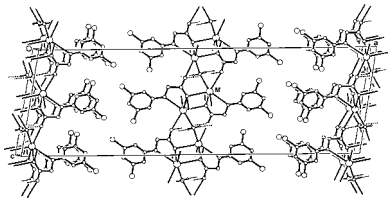
The two-dimensional coordination polymeric structures of the hydrated potassium and rubidium salts of (3,5-dichlorophenoxy)acetic acid (3,5-D), namely, poly[μ-aqua-bis[μ_3-2-(3,5-dichlorophenoxy)acetato]dipotassium], $[K_2(C_8H_5Cl_2O_3)_2(H_2O)]_n$, and poly[$\mu$-aqua-bis[$\mu_3$-2-(3,5-dichlorophenoxy)-acetato]dirubidium], $[Rb_2(C_8H_5Cl_2O_3)_2(H_2O)]_n$, respectively, have been determined and are described. The two compounds are isotypic and the polymeric structure is based on centrosymmetric dinuclear bridged complex units. The irregular six-coordination about the alkali cations comprises a bridging water molecule lying on a twofold rotation axis, the phenoxy O-atom donor and a triple bridging carboxylate O atom of the oxoacetate side chain of the 3,5-D ligand, and the second carboxyate O-atom donor also bridging. The K—O and Rb—O bond-length ranges are 2.7238 (15)–2.9459 (14) and 2.832 (2)–3.050 (2) Å, respectively, and the K···K and Rb···Rb separations in the dinuclear units are 4.0214 (7) and 4.1289 (6) Å, respectively. Within the layers which lie parallel to (100), the coordinating water molecule forms an O—H···O hydrogen bond to the single bridging carboxylate O atom.

1. Chemical context

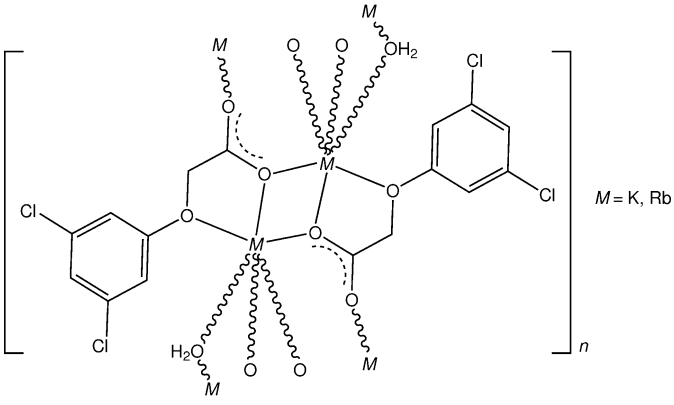
The phenoxyacetic acids are a particularly useful series of compounds since certain members having specific ring-substituents have herbicidal activity, resulting in their being used commercially. Of these, the most common have been the chlorine-substituted analogues (2,4-dichlorophenoxy)acetic acid (2,4-D), (2,4,5-trichlorophenoxy)acetic acid (2,4,5-T) and (4-chloro-2-methylphenoxy)acetic acid (MCPA) (Zumdahl, 2010). As such, the active members have received considerable attention, particularly with respect to health aspects resulting from residual breakdown components after environmental exposure. Compounds formed from their reaction with a wide range of metals have provided a significant number of crystal structures, *e.g.* for 2,4-D, there are 60 examples of metal complexes, contained in the Cambridge Structural Database (CSD; Groom & Allen, 2014), *e.g.* with Ca^{II} (Song *et al.*, 2002) and with Zn^{II} (Kobylecka *et al.*, 2012).

Metal complex formation with the phenoxyacetic acids has been facilitated by their versatility as ligands, showing various interactive modes with common metals including monodentate and bidentate-bridging coordinations involving the $O_{carboxyl}$, $O^1_{phenoxy}$ [$(O,O)^1$] chelate interaction, first reported for the monomeric copper(II) phenoxyacetate complex (Prout *et al.*, 1968) and also found in the potassium–2,4-D salt (Kennard *et al.*, 1983) as well as in the caesium complexes with 4-fluorophenoxyacetate and (4-chloro-2-methyl)phenoxy-acetate (Smith, 2015*a*). In the caesium complex-adduct with 2,4-D (Smith & Lynch, 2014), a tridentate chelate interaction



variant is found which includes, in addition to the O,O^1-chelate, a Cs—Cl bond to the *ortho*-Cl ring substituent of the ligand. Only occasional examples of the bidentate carboxylate O,O'-chelate interaction are found, *e.g.* with the previously mentioned caesium 4-fluorophenoxyacetate.

However, examples of structures of alkali metal salts of the phenoxyacetic acids are not common in the crystallographic literature, comprising, apart from the previously mentioned examples, the following: sodium phenoxyacetate hemihydrate (Prout *et al.*, 1971; Evans *et al.*, 2001), anhydrous caesium phenoxyacetate (Smith, 2014*a*), the lithium, rubidium and caesium complexes of 2,4-D (Smith, 2015*a*), caesium *o*-phenylenedioxydiacetate dihydrate (Smith *et al.*, 1989) and the lithium salts of (2-chlorophenoxy)acetic acid (O'Reilly *et al.*, 1987), (2-carbamoylphenoxy)acetic acid (Mak *et al.*, 1986) and (2-carboxyphenoxy)acetic acid (Smith *et al.*, 1986).



To investigate the nature of the coordination complex structures formed in the potassium and rubidium salts of the 2,4-D isomer, reactions of (3,5-dichlorophenoxy)acetic acid (3,5-D) with K_2CO_3 and Rb_2CO_3 in aqueous ethanol were carried out, affording the isotypic polymeric title compounds $[K_2(C_8H_5Cl_2O_3)_2(H_2O)]_n$, (I), and $[Rb_2(C_8H_5Cl_2O_3)_2(H_2O)]_n$, (II), and the structures are reported herein.

Table 1
Selected bond lengths (Å) for (I).

K1—O1*W*	2.7947 (15)	K1—O13^{i}	2.7855 (15)
K1—O11	2.9459 (14)	K1—O13^{ii}	2.7462 (13)
K1—O13	2.7238 (15)	K1—O14^{iii}	2.7309 (16)

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, -y+1, z-\frac{1}{2}$.

Table 2
Selected bond lengths (Å) for (II).

Rb1—O1*W*	2.924 (2)	Rb1—O13^{i}	2.874 (2)
Rb1—O11	3.050 (2)	Rb1—O13^{ii}	2.894 (2)
Rb1—O13	2.832 (2)	Rb1—O14^{iii}	2.842 (2)

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, -y+1, z-\frac{1}{2}$.

2. Structural commentary

The hydrated complexes (I) and (II) are isotypic and are described conjointly. Each comprises a centrosymmetric dinuclear repeating unit (Fig. 1) in which the irregular six-coordination about the K^+ or Rb^+ cations consists of a bidentate $O_{carboxylate}$ (O13), $O_{phenoxy}$ (O11) chelate interaction (Fig. 2), three bridging carboxylate (O13^{i}, O13^{ii}, O14^{iii}; for symmetry codes, see Table 1) interactions and a single bridging water molecule (O1*W*) lying on a twofold rotation axis. The comparative *M*—O bond length range for the two metals (Tables 1 and 2) is 2.7238 (15)–2.9459 (14) Å (K) and 2.832 (2)–3.050 (2) Å (Rb), for the two O-atom donors in the (O:O^1)-chelate interaction (O13 and O11, respectively).

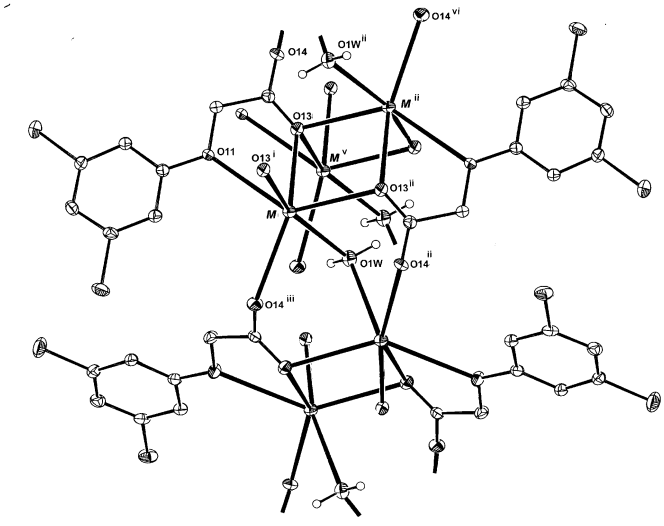


Figure 1
A view of the partially expanded polymeric extension of the structures of (I) and (II), shown with 30% probability ellipsoids (with data taken from the potassium structure). [See Table 1 for symmetry codes; additionally: (vi) $x-1, y, z$; (vii) $x, y-1, z$.]

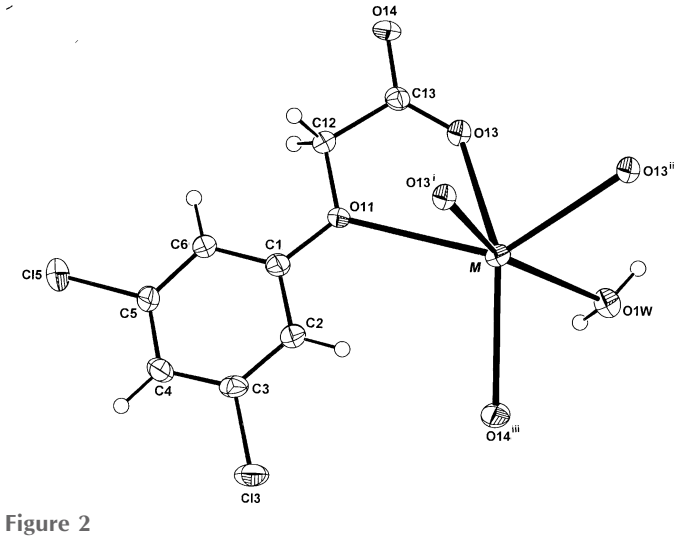


Figure 2
The molecular configuration and atom-numbering scheme for the isomeric K and Rb complexes with 3,5-D [(I) and (II)], with displacement ellipsoids drawn at the 40% probability level (with data taken from the potassium structure). For symmetry codes, see Table 1.

Table 3
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O14^{iv}	0.85 (2)	1.90 (2)	2.750 (2)	174 (2)

Symmetry code: (iv) $-x+1, -y, -z+1$.

Table 4
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O14^{iv}	0.89 (3)	1.87 (3)	2.750 (3)	171 (5)

Symmetry code: (iv) $-x+1, -y, -z+1$.

Two-dimensional coordination polymeric structures are generated, lying parallel to (100) (Fig. 3), in which the core sheet comprises the M—O complex network with the aromatic rings of the ligands peripherally located between the layers. Within the layers there are a number of short metal···metal contacts, the shortest being across an inversion centre [K···K^{ii} = 4.0214 (7) Å and Rb···Rb^{ii} = 4.1289 (6) Å], the longest being K···K^{vi} = 4.3327 (5) Å and Rb···Rb^{vi} = 4.5483 (5) Å [symmetry codes: (ii) $-x+1, -y+1, -z+1$; (vi) $-x+1, y, -z+\frac{1}{2}$]. No inter-ring π–π interactions are found in either (I) or (II), the minimum ring-centroid separations being 4.3327 (1) Å in (I) and 4.3302 (3) Å in (II), (the *b*-axis dimensions). The coordinating water molecules on the twofold rotation axes are involved in intra-layer bridging O—H···O$_{carboxyl}$ hydrogen-bonding interactions (with O14 and O14^{iv}) (Tables 3 and 4).

The 3,5-D anions in both (I) and (II) adopt the *anti-periplanar* conformation with the defining oxoacetate side chain torsion angles C1—O11—C12—O13 of −171.55 (15) and −172.4 (2)° for (I), (II), respectively, that are similar to −172.4 (3)° in the ammonium salt (Smith, 2015*b*). These values contrast with the value in the 2:1 3,5-D adduct with 4,4′-biphenyl [−71.6 (3)°] (*synclinal*) (Lynch *et al.*, 2003).

The present isotypic potassium and rubidium salts of (3,5-dichlorophenoxy)acetic acid provide an example of isotypism which extends to the ammonium salt (Smith, 2015*b*). Isotypism is also found in the analogous NH_4^+, K^+ and Rb^+ hemihydrate salts of isomeric 2,4-D (Table 5). It may also be possible that a similar series exists with MCPA for which the structure of only the ammonium hemihydrate salt (NH_4^+ MCPA$^-$·0.5H$_2$O) is known (Smith, 2014*b*). It is of note that the sodium salts are not included in the sets, the structures for which are not known.

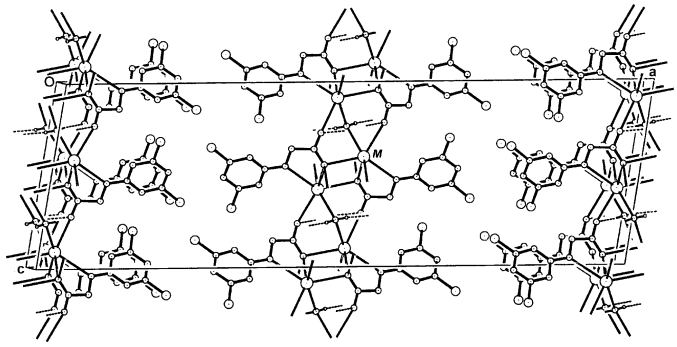


Figure 3
The packing of the layered structure of compounds (I) and (II) in the unit cell, viewed approximately along [010]. Non-associated H atoms have been omitted.

3. Synthesis and crystallization

Compounds (I) and (II) were synthesized by the addition of 0.5 mmol of K_2CO_3 (65 mg) [for (I)] or Rb_2CO_3 (115 mg) (for (II)] to a hot solution of (3,5-dichlorophenoxy)acetic acid (3,5-D) (220 mg) in 10 ml of 50% (*v*/*v*) ethanol/water. After heating for 5 min, partial room temperature evaporation of the solutions gave in all two cases, colourless needles from which specimens were cleaved for the X-ray analyses.

4. Refinement details

Crystal data, data collection and structure refinement details for (I) and (II) are summarized in Table 6. Hydrogen atoms were placed in calculated positions [C—H$_{aromatic}$ = 0.95 Å or C—H$_{methylene}$ = 0.99 Å] and were allowed to ride in the refinements, with U_{iso}(H) = 1.2U_{eq}(C). The water H-atom in both structures was located in a difference Fourier map and was allowed to ride in the refinements with an O—H distance restraint of 0.90±0.02 Å and with U_{iso}(H) = 1.5U_{eq}(O).

Table 5
Comparative cell data (Å, °, Å^3) for NH_4^+, K^+ and Rb^+ salts of (3,5-dichlorophenoxy)acetic acid (3,5-D), (2,4-dichlorophenoxy)acetic acid (2,4-D) and (4-chloro-2-methylphenoxy)acetic acid (MCPA).

Cell parameters	NH_4^+3,5-D$^-$·0.5H$_2$O	K^+3,5-D$^-$·0.5H$_2$O	Rb^+3,5-D$^-$·0.5H$_2$O	NH_4^+2,4-D$^-$·0.5H$_2$O	K^+2,4-D$^-$·0.5H$_2$O	Rb^+2,4-D$^-$·0.5H$_2$O	NH_4^+MCPA$^-$·0.5H$_2$O
a	39.818 (3)	39.274 (2)	39.641 (3)	39.3338 (8)	36.80 (1)	37.254 (2)	38.0396 (9)
b	4.3340 (4)	4.3327 (3)	4.3302 (3)	4.3889 (9)	4.339 (1)	4.3589 (3)	4.456 (5)
c	12.7211 (8)	12.4234 (10)	12.8607 (8)	12.900 (3)	12.975 (7)	13.238 (1)	12.944 (5)
β (°)	98.098 (5)	99.363 (6)	98.404 (5)	103.83 (3)	102.03 (4)	103.231 (7)	104.575 (5)
V	2178.4 (5)	2085.8 (3)	2183.9 (3)	2074.7 (8)	2026 (2)	2092.6 (3)	2123 (3)
Z	8	8	8	8	8	8	8
Space group	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*
Reference	Smith (2015*b*)	This work (I)	This work (II)	Liu *et al.* (2009)	Smith (2015*a*)	Smith (2015*a*)	Smith (2014*b*)

Table 6
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$[K_2(C_8H_5Cl_2O_3)_2(H_2O)]$	$[Rb_2(C_8H_5Cl_2O_3)_2(H_2O)]$
M_r	536.26	629.00
Crystal system, space group	Monoclinic, *C*2/*c*	Monoclinic, *C*2/*c*
Temperature (K)	200	200
a, *b*, *c* (Å)	39.274 (2), 4.3327 (3), 12.4234 (10)	39.641 (3), 4.3302 (3), 12.8607 (8)
β (°)	99.363 (6)	98.404 (5)
V (Å^3)	2085.8 (3)	2183.9 (3)
Z	4	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	1.00	5.01
Crystal size (mm)	0.45 × 0.12 × 0.04	0.40 × 0.12 × 0.04
Data collection		
Diffractometer	Oxford Diffraction Gemini-S CCD detector	Oxford Diffraction Gemini-S CCD detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2013)	Multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min}, T_{max}	0.774, 0.980	0.369, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6745, 2061, 1824	7520, 2152, 1910
R_{int}	0.035	0.055
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.031, 0.076, 1.07	0.040, 0.095, 1.06
No. of reflections	2061	2152
No. of parameters	135	136
No. of restraints	1	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.25	0.98, −1.00

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SIR92* (Altomare *et al.*, 1993), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009).

Acknowledgements

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supporting information

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Crystal structures of the potassium and rubidium salts of (3,5-dichlorophenoxy)-acetic acid: two isotypic coordination polymers

Graham Smith

Computing details

For both compounds, data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO* (Agilent, 2013); data reduction: *CrysAlis PRO* (Agilent, 2013). Program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993) for (I); *SHELXS97* (Sheldrick, 2008) for (II). For both compounds, program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

(I) Poly[μ-aqua-bis[μ_3-2-(3,5-dichlorophenoxy)acetato]dipotassium]

Crystal data

$[K_2(C_8H_5Cl_2O_3)_2(H_2O)]$
M_r = 536.26
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 39.274 (2) Å
b = 4.3327 (3) Å
c = 12.4234 (10) Å
β = 99.363 (6)°
V = 2085.8 (3) Å^3
Z = 4
F(000) = 1080
D_x = 1.708 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2400 reflections
θ = 4.2–28.6°
μ = 1.00 mm^{-1}
T = 200 K
Flat prism, colourless
0.45 × 0.12 × 0.04 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
Detector resolution: 16.077 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.774, T_{max} = 0.980
6745 measured reflections
2061 independent reflections
1824 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 26.0°, θ_{min} = 3.2°
h = −48→47
k = −5→5
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.076
S = 1.07
2061 reflections
135 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.706P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
K1	0.53071 (1)	0.71864 (10)	0.40994 (4)	0.0253 (1)
Cl3	0.66484 (1)	1.12106 (12)	0.30636 (5)	0.0351 (2)
Cl5	0.72749 (1)	0.44252 (15)	0.64380 (5)	0.0436 (2)
O1W	0.50000	0.3066 (5)	0.25000	0.0301 (7)
O11	0.59608 (3)	0.5041 (3)	0.53873 (12)	0.0279 (4)
O13	0.53561 (3)	0.2277 (3)	0.54855 (12)	0.0279 (4)
O14	0.55253 (4)	0.0910 (3)	0.72297 (12)	0.0317 (5)
C1	0.62867 (5)	0.5876 (4)	0.52303 (17)	0.0226 (6)
C2	0.63030 (5)	0.7874 (4)	0.43626 (17)	0.0243 (6)
C3	0.66234 (5)	0.8758 (4)	0.41548 (17)	0.0250 (6)
C4	0.69289 (5)	0.7753 (5)	0.47741 (18)	0.0286 (6)
C5	0.69014 (5)	0.5791 (5)	0.56273 (18)	0.0268 (6)
C6	0.65879 (5)	0.4817 (5)	0.58735 (17)	0.0242 (6)
C12	0.59359 (5)	0.3273 (5)	0.63485 (17)	0.0276 (6)
C13	0.55716 (5)	0.2100 (4)	0.63421 (17)	0.0228 (6)
H1W	0.4837 (5)	0.189 (5)	0.263 (2)	0.0340*
H2	0.60980	0.86110	0.39240	0.0290*
H4	0.71470	0.83880	0.46170	0.0340*
H6	0.65780	0.34570	0.64670	0.0290*
H121	0.60060	0.45750	0.70020	0.0330*
H122	0.60960	0.14980	0.63920	0.0330*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0223 (2)	0.0305 (2)	0.0223 (3)	−0.0004 (2)	0.0016 (2)	−0.0001 (2)
Cl3	0.0440 (3)	0.0342 (3)	0.0282 (3)	−0.0098 (2)	0.0095 (3)	0.0029 (2)
Cl5	0.0188 (3)	0.0630 (4)	0.0457 (4)	−0.0017 (3)	−0.0046 (2)	0.0085 (3)
O1W	0.0230 (11)	0.0293 (11)	0.0381 (14)	0.0000	0.0051 (10)	0.0000
O11	0.0163 (7)	0.0415 (8)	0.0251 (8)	−0.0026 (6)	0.0011 (6)	0.0101 (7)
O13	0.0197 (7)	0.0353 (8)	0.0266 (8)	−0.0036 (6)	−0.0028 (6)	−0.0003 (7)
O14	0.0293 (8)	0.0418 (9)	0.0251 (9)	−0.0062 (7)	0.0075 (7)	0.0028 (7)

C1	0.0185 (10)	0.0278 (10)	0.0214 (11)	−0.0023 (8)	0.0029 (8)	−0.0037 (9)
C2	0.0228 (10)	0.0267 (10)	0.0226 (11)	−0.0002 (8)	0.0015 (8)	−0.0016 (9)
C3	0.0302 (11)	0.0243 (10)	0.0211 (11)	−0.0049 (9)	0.0061 (9)	−0.0034 (9)
C4	0.0222 (10)	0.0348 (11)	0.0297 (12)	−0.0077 (9)	0.0070 (9)	−0.0070 (10)
C5	0.0180 (10)	0.0338 (11)	0.0266 (12)	−0.0019 (8)	−0.0023 (8)	−0.0039 (9)
C6	0.0206 (10)	0.0303 (10)	0.0213 (11)	−0.0027 (8)	0.0021 (8)	−0.0005 (9)
C12	0.0232 (11)	0.0384 (11)	0.0200 (11)	−0.0054 (9)	0.0002 (9)	0.0063 (9)
C13	0.0196 (10)	0.0233 (9)	0.0256 (12)	0.0003 (8)	0.0039 (9)	−0.0039 (9)

Geometric parameters (Å, º)

K1—O1W	2.7947 (15)	O1W—H1W^{iv}	0.85 (2)
K1—O11	2.9459 (14)	C1—C6	1.393 (3)
K1—O13	2.7238 (15)	C1—C2	1.392 (3)
K1—O13^{i}	2.7855 (15)	C2—C3	1.379 (3)
K1—O13^{ii}	2.7462 (13)	C3—C4	1.386 (3)
K1—O14^{iii}	2.7309 (16)	C4—C5	1.377 (3)
Cl3—C3	1.738 (2)	C5—C6	1.382 (3)
Cl5—C5	1.742 (2)	C12—C13	1.517 (3)
O11—C1	1.374 (2)	C2—H2	0.9500
O11—C12	1.435 (3)	C4—H4	0.9500
O13—C13	1.250 (2)	C6—H6	0.9500
O14—C13	1.257 (2)	C12—H121	0.9900
O1W—H1W	0.85 (2)	C12—H122	0.9900
O1W—K1—O11	114.95 (4)	H1W—O1W—H1W^{iv}	107 (2)
O1W—K1—O13	85.90 (5)	K1^{iv}—O1W—H1W^{iv}	119.8 (16)
O1W—K1—O13^{i}	157.48 (4)	O11—C1—C2	115.78 (17)
O1W—K1—O13^{ii}	82.81 (3)	O11—C1—C6	123.74 (18)
O1W—K1—O14^{iii}	75.35 (4)	C2—C1—C6	120.48 (18)
O11—K1—O13	56.26 (4)	C1—C2—C3	118.42 (18)
O11—K1—O13^{i}	87.00 (4)	C2—C3—C4	122.86 (19)
O11—K1—O13^{ii}	133.96 (4)	Cl3—C3—C4	118.13 (15)
O11—K1—O14^{iii}	101.01 (4)	Cl3—C3—C2	119.01 (15)
O13—K1—O13^{i}	103.70 (4)	C3—C4—C5	116.88 (18)
O13—K1—O13^{ii}	85.35 (4)	Cl5—C5—C4	119.39 (16)
O13—K1—O14^{iii}	140.71 (4)	C4—C5—C6	122.91 (19)
O13^{i}—K1—O13^{ii}	77.83 (4)	Cl5—C5—C6	117.71 (17)
O13^{i}—K1—O14^{iii}	106.68 (4)	C1—C6—C5	118.45 (19)
O13^{ii}—K1—O14^{iii}	124.93 (5)	O11—C12—C13	111.48 (16)
K1—O1W—K1^{iv}	100.60 (7)	O13—C13—C12	119.43 (18)
K1—O11—C1	126.11 (11)	O14—C13—C12	113.81 (18)
K1—O11—C12	116.68 (10)	O13—C13—O14	126.70 (18)
C1—O11—C12	116.72 (15)	C1—C2—H2	121.00
K1—O13—C13	123.69 (11)	C3—C2—H2	121.00
K1—O13—K1^{v}	103.70 (5)	C3—C4—H4	122.00
K1—O13—K1^{ii}	94.65 (4)	C5—C4—H4	122.00
K1^{v}—O13—C13	116.55 (11)	C1—C6—H6	121.00

K1^{ii}—O13—C13	112.14 (12)	C5—C6—H6	121.00
K1^{v}—O13—K1^{ii}	102.18 (4)	O11—C12—H121	109.00
K1^{vi}—O14—C13	137.09 (12)	O11—C12—H122	109.00
K1^{iv}—O1W—H1W	105.4 (15)	C13—C12—H121	109.00
K1—O1W—H1W	119.8 (16)	C13—C12—H122	109.00
K1—O1W—H1W^{iv}	105.4 (15)	H121—C12—H122	108.00
O11—K1—O1W—K1^{iv}	−146.99 (3)	O13—K1—O13^{ii}—K1^{ii}	−0.02 (5)
O13—K1—O1W—K1^{iv}	163.37 (3)	O13—K1—O13^{ii}—C13^{ii}	−129.34 (12)
O1W—K1—O11—C1	99.66 (13)	O11—K1—O14^{iii}—C13^{iii}	87.4 (2)
O1W—K1—O11—C12	−88.68 (13)	O13—K1—O14^{iii}—C13^{iii}	38.4 (2)
O13—K1—O11—C1	165.74 (15)	K1—O11—C1—C2	−1.4 (2)
O13—K1—O11—C12	−22.60 (12)	K1—O11—C1—C6	179.21 (14)
O13^{i}—K1—O11—C1	−85.59 (14)	C12—O11—C1—C2	−173.08 (17)
O13^{i}—K1—O11—C12	86.08 (12)	C12—O11—C1—C6	7.6 (3)
O13^{ii}—K1—O11—C1	−155.47 (13)	K1—O11—C12—C13	15.98 (19)
O13^{ii}—K1—O11—C12	16.20 (14)	C1—O11—C12—C13	−171.55 (15)
O14^{iii}—K1—O11—C1	20.83 (14)	K1—O13—C13—O14	143.75 (15)
O14^{iii}—K1—O11—C12	−167.51 (12)	K1—O13—C13—C12	−39.2 (2)
O1W—K1—O13—C13	156.32 (14)	K1^{v}—O13—C13—O14	−85.6 (2)
O1W—K1—O13—K1^{v}	20.65 (4)	K1^{v}—O13—C13—C12	91.41 (17)
O1W—K1—O13—K1^{ii}	−83.10 (4)	K1^{ii}—O13—C13—O14	31.6 (2)
O11—K1—O13—C13	32.52 (14)	K1^{ii}—O13—C13—C12	−151.35 (14)
O11—K1—O13—K1^{v}	−103.16 (5)	K1^{vi}—O14—C13—O13	−90.6 (2)
O11—K1—O13—K1^{ii}	153.10 (6)	K1^{vi}—O14—C13—C12	92.3 (2)
O13^{i}—K1—O13—C13	−44.32 (15)	O11—C1—C2—C3	−179.06 (16)
O13^{i}—K1—O13—K1^{v}	179.98 (9)	C6—C1—C2—C3	0.3 (3)
O13^{i}—K1—O13—K1^{ii}	76.26 (5)	O11—C1—C6—C5	179.20 (18)
O13^{ii}—K1—O13—C13	−120.58 (14)	C2—C1—C6—C5	−0.1 (3)
O13^{ii}—K1—O13—K1^{v}	103.75 (5)	C1—C2—C3—Cl3	179.16 (14)
O13^{ii}—K1—O13—K1^{ii}	0.02 (8)	C1—C2—C3—C4	−0.3 (3)
O14^{iii}—K1—O13—C13	95.53 (16)	Cl3—C3—C4—C5	−179.45 (16)
O14^{iii}—K1—O13—K1^{v}	−40.15 (8)	C2—C3—C4—C5	0.0 (3)
O14^{iii}—K1—O13—K1^{ii}	−143.89 (6)	C3—C4—C5—Cl5	179.79 (16)
O11—K1—O13^{i}—K1^{i}	125.82 (4)	C3—C4—C5—C6	0.2 (3)
O11—K1—O13^{i}—C13^{i}	−13.64 (13)	Cl5—C5—C6—C1	−179.71 (16)
O13—K1—O13^{i}—K1^{i}	180.00 (4)	C4—C5—C6—C1	−0.2 (3)
O13—K1—O13^{i}—C13^{i}	40.53 (13)	O11—C12—C13—O13	12.0 (2)
O11—K1—O13^{ii}—K1^{ii}	−31.51 (7)	O11—C12—C13—O14	−170.65 (16)
O11—K1—O13^{ii}—C13^{ii}	−160.85 (11)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+1, *z*−1/2; (iv) −*x*+1, *y*, −*z*+1/2; (v) *x*, *y*−1, *z*; (vi) *x*, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O14^{vii}	0.85 (2)	1.90 (2)	2.750 (2)	174 (2)

Symmetry code: (vii) −*x*+1, −*y*, −*z*+1.

(II) Poly[μ-aqua-bis[μ_3-(3,5-dichlorophenoxy)acetato]dirubidium]

Crystal data

$[Rb_2(C_8H_5Cl_2O_3)_2(H_2O)]$
M_r = 629.00
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 39.641 (3) Å
b = 4.3302 (3) Å
c = 12.8607 (8) Å
β = 98.404 (5)°
V = 2183.9 (3) Å^3
Z = 4
F(000) = 1224
D_x = 1.913 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2435 reflections
θ = 3.6–28.3°
μ = 5.01 mm^{-1}
T = 200 K
Prism, colourless
0.40 × 0.12 × 0.04 mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
Detector resolution: 16.077 pixels mm^{-1}
ω–scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.369, T_{max} = 0.980
7520 measured reflections
2152 independent reflections
1910 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 26.0°, θ_{min} = 3.2°
h = −45→48
k = −5→5
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.095
S = 1.06
2152 reflections
136 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Rb1	0.53252 (1)	0.71425 (8)	0.41106 (2)	0.0271 (1)
Cl3	0.66575 (3)	1.1071 (2)	0.31320 (7)	0.0394 (3)
Cl5	0.72802 (2)	0.4700 (3)	0.64713 (9)	0.0510 (4)
O1W	0.50000	0.2897 (8)	0.25000	0.0336 (12)

O11	0.59805 (6)	0.4938 (6)	0.54449 (18)	0.0312 (8)
O13	0.53789 (6)	0.2205 (5)	0.5570 (2)	0.0295 (8)
O14	0.55505 (6)	0.0734 (6)	0.72371 (19)	0.0341 (8)
C1	0.63017 (8)	0.5832 (8)	0.5286 (3)	0.0255 (11)
C2	0.63168 (10)	0.7780 (8)	0.4420 (3)	0.0278 (11)
C3	0.66324 (10)	0.8701 (8)	0.4215 (3)	0.0284 (11)
C4	0.69371 (11)	0.7828 (8)	0.4829 (3)	0.0327 (12)
C5	0.69102 (9)	0.5914 (9)	0.5678 (3)	0.0302 (11)
C6	0.66010 (8)	0.4923 (8)	0.5924 (3)	0.0267 (11)
C12	0.59553 (9)	0.3198 (8)	0.6376 (3)	0.0285 (11)
C13	0.55928 (9)	0.1991 (8)	0.6381 (3)	0.0243 (11)
H1W	0.4832 (8)	0.172 (8)	0.266 (4)	0.0510*
H2	0.61150	0.84410	0.39880	0.0330*
H4	0.71520	0.85090	0.46730	0.0390*
H6	0.65920	0.36420	0.65190	0.0320*
H121	0.60210	0.45220	0.70000	0.0340*
H122	0.61160	0.14340	0.64200	0.0340*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.0270 (2)	0.0340 (2)	0.0204 (2)	0.0005 (1)	0.0035 (2)	0.0014 (1)
Cl3	0.0502 (6)	0.0428 (6)	0.0275 (5)	−0.0119 (5)	0.0132 (5)	0.0037 (4)
Cl5	0.0231 (5)	0.0802 (8)	0.0474 (6)	−0.0029 (5)	−0.0022 (5)	0.0124 (6)
O1W	0.028 (2)	0.034 (2)	0.039 (2)	0.0000	0.0057 (19)	0.0000
O11	0.0205 (13)	0.0506 (16)	0.0227 (13)	−0.0044 (11)	0.0038 (11)	0.0129 (12)
O13	0.0245 (14)	0.0378 (14)	0.0255 (14)	−0.0029 (10)	0.0013 (12)	−0.0011 (11)
O14	0.0317 (14)	0.0491 (16)	0.0232 (13)	−0.0085 (13)	0.0100 (12)	0.0059 (12)
C1	0.0249 (19)	0.0317 (19)	0.0205 (18)	−0.0028 (16)	0.0051 (16)	−0.0045 (16)
C2	0.027 (2)	0.035 (2)	0.0215 (19)	−0.0002 (15)	0.0038 (17)	−0.0013 (15)
C3	0.037 (2)	0.0300 (19)	0.0194 (18)	−0.0075 (17)	0.0084 (17)	−0.0052 (15)
C4	0.028 (2)	0.044 (2)	0.028 (2)	−0.0104 (17)	0.0106 (18)	−0.0055 (17)
C5	0.0238 (19)	0.042 (2)	0.0241 (18)	−0.0042 (17)	0.0013 (16)	−0.0036 (17)
C6	0.0244 (19)	0.035 (2)	0.0207 (18)	−0.0020 (15)	0.0036 (15)	−0.0013 (16)
C12	0.025 (2)	0.040 (2)	0.0200 (18)	−0.0040 (16)	0.0018 (16)	0.0041 (16)
C13	0.024 (2)	0.0269 (18)	0.0231 (19)	0.0007 (15)	0.0071 (17)	−0.0048 (15)

Geometric parameters (Å, º)

Rb1—O1W	2.924 (2)	O1W—H1W^{iv}	0.89 (3)
Rb1—O11	3.050 (2)	C1—C6	1.397 (5)
Rb1—O13	2.832 (2)	C1—C2	1.405 (5)
Rb1—O13^{i}	2.874 (2)	C2—C3	1.375 (6)
Rb1—O13^{ii}	2.894 (2)	C3—C4	1.395 (6)
Rb1—O14^{iii}	2.842 (2)	C4—C5	1.387 (5)
Cl3—C3	1.745 (4)	C5—C6	1.378 (5)
Cl5—C5	1.741 (4)	C12—C13	1.530 (5)
O11—C1	1.374 (4)	C2—H2	0.9500

O11—C12	1.431 (4)	C4—H4	0.9500
O13—C13	1.248 (5)	C6—H6	0.9500
O14—C13	1.261 (4)	C12—H121	0.9900
O1W—H1W	0.89 (3)	C12—H122	0.9900

O1W—Rb1—O11	116.93 (7)	H1W—O1W—H1W^{iv}	110 (3)
O1W—Rb1—O13	88.71 (7)	Rb1^{iv}—O1W—H1W^{iv}	118 (3)
O1W—Rb1—O13^{i}	157.69 (6)	O11—C1—C2	115.8 (3)
O1W—Rb1—O13^{ii}	80.06 (5)	O11—C1—C6	124.0 (3)
O1W—Rb1—O14^{iii}	76.32 (6)	C2—C1—C6	120.3 (3)
O11—Rb1—O13	54.24 (7)	C1—C2—C3	118.1 (3)
O11—Rb1—O13^{i}	84.01 (7)	C2—C3—C4	123.3 (4)
O11—Rb1—O13^{ii}	135.28 (7)	Cl3—C3—C4	117.8 (3)
O11—Rb1—O14^{iii}	103.36 (7)	Cl3—C3—C2	118.9 (3)
O13—Rb1—O13^{i}	98.73 (7)	C3—C4—C5	116.6 (4)
O13—Rb1—O13^{ii}	87.72 (7)	Cl5—C5—C4	119.1 (3)
O13—Rb1—O14^{iii}	143.47 (7)	C4—C5—C6	122.7 (4)
O13^{i}—Rb1—O13^{ii}	79.26 (7)	Cl5—C5—C6	118.2 (3)
O13^{i}—Rb1—O14^{iii}	107.73 (7)	C1—C6—C5	119.0 (3)
O13^{ii}—Rb1—O14^{iii}	121.19 (7)	O11—C12—C13	111.3 (3)
Rb1—O1W—Rb1^{iv}	102.10 (11)	O13—C13—C12	119.7 (3)
Rb1—O11—C1	124.0 (2)	O14—C13—C12	113.3 (3)
Rb1—O11—C12	118.55 (19)	O13—C13—O14	126.9 (3)
C1—O11—C12	116.9 (3)	C1—C2—H2	121.00
Rb1—O13—C13	125.9 (2)	C3—C2—H2	121.00
Rb1—O13—Rb1^{v}	98.73 (8)	C3—C4—H4	122.00
Rb1—O13—Rb1^{ii}	92.28 (7)	C5—C4—H4	122.00
Rb1^{v}—O13—C13	117.8 (2)	C1—C6—H6	121.00
Rb1^{ii}—O13—C13	116.1 (2)	C5—C6—H6	120.00
Rb1^{v}—O13—Rb1^{ii}	100.74 (7)	O11—C12—H121	109.00
Rb1^{vi}—O14—C13	134.3 (2)	O11—C12—H122	109.00
Rb1^{iv}—O1W—H1W	105 (3)	C13—C12—H121	109.00
Rb1—O1W—H1W	118 (3)	C13—C12—H122	109.00
Rb1—O1W—H1W^{iv}	105 (3)	H121—C12—H122	108.00

O11—Rb1—O1W—Rb1^{iv}	−149.55 (5)	O13—Rb1—O13^{ii}—Rb1^{ii}	0.00 (7)
O13—Rb1—O1W—Rb1^{iv}	162.30 (5)	O13—Rb1—O13^{ii}—C13^{ii}	−132.3 (2)
O1W—Rb1—O11—C1	101.0 (2)	O11—Rb1—O14^{iii}—C13^{iii}	88.7 (3)
O1W—Rb1—O11—C12	−87.7 (2)	O13—Rb1—O14^{iii}—C13^{iii}	42.2 (4)
O13—Rb1—O11—C1	167.6 (3)	Rb1—O11—C1—C2	−2.7 (4)
O13—Rb1—O11—C12	−21.0 (2)	Rb1—O11—C1—C6	177.2 (3)
O13^{i}—Rb1—O11—C1	−87.1 (2)	C12—O11—C1—C2	−174.3 (3)
O13^{i}—Rb1—O11—C12	84.3 (2)	C12—O11—C1—C6	5.7 (5)
O13^{ii}—Rb1—O11—C1	−155.3 (2)	Rb1—O11—C12—C13	15.6 (3)
O13^{ii}—Rb1—O11—C12	16.1 (3)	C1—O11—C12—C13	−172.4 (3)
O14^{iii}—Rb1—O11—C1	19.7 (3)	Rb1—O13—C13—O14	147.4 (3)
O14^{iii}—Rb1—O11—C12	−168.9 (2)	Rb1—O13—C13—C12	−35.8 (4)
O1W—Rb1—O13—C13	155.0 (3)	Rb1^{v}—O13—C13—O14	−86.3 (4)

O1W—Rb1—O13—Rb1^{v}	21.13 (6)	Rb1^{v}—O13—C13—C12	90.5 (3)
O1W—Rb1—O13—Rb1^{ii}	−80.10 (5)	Rb1^{ii}—O13—C13—O14	33.2 (4)
O11—Rb1—O13—C13	29.9 (3)	Rb1^{ii}—O13—C13—C12	−150.0 (2)
O11—Rb1—O13—Rb1^{v}	−103.93 (9)	Rb1^{vi}—O14—C13—O13	−90.5 (4)
O11—Rb1—O13—Rb1^{ii}	154.83 (10)	Rb1^{vi}—O14—C13—C12	92.5 (3)
O13^{i}—Rb1—O13—C13	−46.2 (3)	O11—C1—C2—C3	−178.9 (3)
O13^{i}—Rb1—O13—Rb1^{v}	179.98 (11)	C6—C1—C2—C3	1.1 (5)
O13^{i}—Rb1—O13—Rb1^{ii}	78.77 (7)	O11—C1—C6—C5	178.8 (3)
O13^{ii}—Rb1—O13—C13	−124.9 (3)	C2—C1—C6—C5	−1.3 (5)
O13^{ii}—Rb1—O13—Rb1^{v}	101.23 (7)	C1—C2—C3—Cl3	179.0 (3)
O13^{ii}—Rb1—O13—Rb1^{ii}	0.00 (7)	C1—C2—C3—C4	−0.7 (6)
O14^{iii}—Rb1—O13—C13	90.3 (3)	Cl3—C3—C4—C5	−179.3 (3)
O14^{iii}—Rb1—O13—Rb1^{v}	−43.54 (14)	C2—C3—C4—C5	0.5 (5)
O14^{iii}—Rb1—O13—Rb1^{ii}	−144.77 (9)	C3—C4—C5—Cl5	179.4 (3)
O11—Rb1—O13^{i}—Rb1^{i}	127.64 (8)	C3—C4—C5—C6	−0.7 (6)
O11—Rb1—O13^{i}—C13^{i}	−11.0 (2)	Cl5—C5—C6—C1	−178.9 (3)
O13—Rb1—O13^{i}—Rb1^{i}	179.98 (10)	C4—C5—C6—C1	1.1 (6)
O13—Rb1—O13^{i}—C13^{i}	41.3 (2)	O11—C12—C13—O13	10.0 (4)
O11—Rb1—O13^{ii}—Rb1^{ii}	−29.37 (12)	O11—C12—C13—O14	−172.7 (3)
O11—Rb1—O13^{ii}—C13^{ii}	−161.6 (2)		

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+1, *z*−1/2; (iv) −*x*+1, *y*, −*z*+1/2; (v) *x*, *y*−1, *z*; (vi) *x*, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O14^{vii}	0.89 (3)	1.87 (3)	2.750 (3)	171 (5)

Symmetry code: (vii) −*x*+1, −*y*, −*z*+1.